PCSI

Room Keauhou II - Session PCSI-ThM

Topological Properties II/2D Surfaces IV/New Techniques II

Moderators: Xiaodong Xu, University of Washington, Hidemi Shigekawa, University of Tsukuba

8:30am **PCSI-ThM-1 A Valley Valve and Electron Beam Splitter in Bilayer Graphene**, *J Li, R Zhang, Z Yin, J Zhang,* Penn State University*; K Watanabe, T Taniguchi,* National Institute of Materils Science, Japan*; C Liu,* ***Jun Zhu,*** Penn State University **INVITED**

Conventional CMOS field effect transistors control current transmission by controlling the charge of carriers. The advent of two-dimensional materials with hexagonal crystal symmetry offers a new electronic degree of freedom, namely valley, the manipulation of which could potentially be exploited to develop new paradigms of electronic applications dubbed "Valleytronics". I will discuss our work on realizing a valley valve and tunable electron beam splitter in bilayer graphene[1][2].

In high-quality bilayer graphene, the application of a perpendicular electric field opens a tunable band gap, the sign of which can be reversed by reversing the polarity of the applied E-field. Theory predicts the existence of valley-momentum locked one-dimensional conducting channels at the artificial domain wall of two oppositely gapped bilayer graphene regions[3]. Known as the "kink states", they are hallmarks of the quantum valley Hall effect. The helicity of the kink states can be controlled by the polarity of the applied E-field. This unique attribute allows the design of a novel valve and electron beam splitter, where electrically controlled transmission and guiding of the kink states at a four-way intersection have been proposed [4].

Here, we will show our experiments realizing the kink states in bilayer graphene and the operations of a waveguide, a valley valve and beam splitter. The conductance of the kink states exhibits well-developed plateaus with values close to the expected quantization of $4e^2/h$ at zero magnetic field. We will show the transmission of the kink states in the "on" state of the valve and the expected valley blocking effect in the "off" state of the valve. The on/off ratio is about 800% at B=0 and T=1.5 K. The control of the Fermi level in a magnetic field enables a chirality-based beam splitting mechanism. We demonstrate a continuous tuning of the splitting ratio from 0 to close to 100%. The high quality, in-situ electrical control, and scalabilty of the system open the door to many exciting opportunities in valleytronics and fundamental inquiries.

[1] J. Li, K. Wang, K. J. McFaul, Z. Zern, Y. F. Ren, K. Watanabe, T. Taniguchi, Z. H. Qiao, J. Zhu, Nature Nanotechnology, **11**, 1060 (2016)

[2] J. Li, R.-X. Zhang, Z. Yin, J. Zhang, K. Watanabe, T. Taniguchi, C. Liu, and J. Zhu, A valley valve and electron beam splitter in bilayer graphene, arXiv:1708.02311v1 (2017)

[3] I. Martin, Y. M. Blanter, and A. F. Morpurgo, Topological confinement in bilayer graphene, Physical Review Letters **100**, 036804 (2008)

[4] Z. Qiao, J. Jung, Q. Niu, and A. H. MacDonald, Electronic Highways in Bilayer Graphene, Nano Letters **11**, 3453 (2011)

9:00am **PCSI-ThM-7 Topological Phase Transition and Isostructural Phase Transitionin 1T-TiTe2 Single Crystal Under Pressure**, *Z Zhang,* ***Min Zhang,*** University of Science and Technology of China, China

Trigonal $TiTe_2$ (1T-$TiTe_2$) has been studied for a few decades, showing some novel properties such as the enhanced superconductivity under uniaxial strain and the charge density wave (CDW) transition in monolayer form. However, there has been no experimental exploration for its high pressure behavior. In this work, the pressure-induced phase transitions were investigated by Raman scattering and electric resistivity for 1T-$TiTe_2$ single crystal under high pressure up to 17 GPa at room temperature. The result indicated that 1T-$TiTe_2$ single crystal undergoes three phase transitions at 1.7 GPa, 3 GPa and 8 GPa, respectively. The first-principles calculations manifest that the first two transitions at 1.7 GPa and 3 GPa are accompanied with the band inversion near Fermi level, from which parity analysis show two topological phase transitions occur here. Meanwhile, the structural distortion marked by the calculated c/a minimum was observed and proposed to induce the isostructural phase transition at 8 GPa. The observation of the two topological phase transitions and one isostructural phase transition for 1T-$TiTe_2$ single crystal under high pressure immensely enriches the physical understandings for this material family.

9:05am **PCSI-ThM-8 Chemical Potential Tuning and Strain Engineering in Topological Half-Heusler Thin Films**, ***Shouvik Chatterjee***, *J Logan, N Wilson, H Inbar, T Brown-Heft,* University of California, Santa Barbara*; A Fedorov,* Lawrence Berkeley National Lab*; C Palmstrøm,* University of California, Santa Barbara

Heusler compounds have emerged as an exciting material system where realization of functional and tunable novel topological phases might be possible [1-2]. PtLuSb is one such compound that has recently been shown to host topologically non-trivial surface states [3]. However, the chemical potential was found to lie below the Dirac point of the surface states, consistent with p-type Hall conductivity, in our thin films [4]. One way to shift the chemical potential above the Dirac point is to substitute a few of the platinum (Pt) atoms in PtLuSb with gold (Au), which has one more electron compared to Pt. We have successfully synthesized thin films of Au alloyed PtLuSb with different Au concentrations, up to 50% ($Pt_{0.5}Au_{0.5}$LuSb). Employing a combination of the techniques of angle-resolved photoemission spectroscopy via a UHV vacuum suitcase transfer and *in-situ* scanning tunneling spectroscopy along with *ex-situ* transport measurements we will provide evidence of our ability to tune the chemical potential via substitution alloying in Pt_{x1-x}LuSb thin films.

Furthermore, PtLuSb being a semimetal does not possess a bulk band gap. As a result, exotic transport and thermodynamic properties expected from topological surface states are often obscured by contributions from trivial bulk carriers. In this talk, I will present our efforts to address this issue by synthesizing compressively strained thin films on lattice mismatched substrate that is expected to lift the degeneracy of Γ_8 manifold, thereby opening a bulk band gap.

[1] S. Chadov et al, Nature Mater, 9, 541 (2010)

[2] H. Lin et al, Nature Mater, 9, 546 (2010)

[3] J. A. Logan et al, Nature Commun, 7, 11993 (2015)

[4] S. J. Patel et al, Appl. Phys. Lett., 104, 201603 (2014)

+ Author for correspondence: schatterjee@ucsb.edu

9:10am **PCSI-ThM-9 Spin-dependent Processes of Interfacial Charge Transfer Excitons in Polymer-fullerene Solar Cells**, *Y Puttisong, F Gao, Y Xia, I Buyanova, O Inganäs,* ***Weimin M. Chen,*** Linköping University, Sweden

Efficient solar energy conversion in bulk hetero-junction (BHJ) organic photo-voltaic devices relies on photo-generation of charges at the donor and accepter hetero-interfaces. An important requirement in further improving device efficiency is our understanding of the photo physics of interfacial charge transfer (CT) states - the precursors for charge generation, and their contributions to both charge generation and energy losses. Earlier studies have shown that spin and localization of the interfacial CT states play crucial roles in ultrafast charge generation and the subsequent recombination loss in polymer/fullerene blend systems. However, a direct proof for such roles on the microscopic level is still lacking.

In this work, we focus on the direct probing of the optically-excited lowest CT exciton states (CT_1) and their associated spin-dependent processes in a model polymer/fullerene solar cell based on TQ1/PCBM blends. By combining selective optical excitation and detection with the optically detected magnetic resonance (ODMR) technique, we are able to identify the triplet CT_1 states and the associated spin-spin interaction. With this, we estimate the electron-hole separation of the CT_1 exciton to be about 1 nm, within the physical dimension of a one-polymer-one-fullerene unit. The size of the CT_1 exciton is found to be identical in the blends regardless of the fullerene load and aggregation that are known to affect the degree of delocalization of CT excited states. We therefore conclude that the exciton localization of the CT_1 state is not responsible for the observed different efficiency of the solar cells with different fullerene loads. In addition, we provide direct evidence that CT_1 can mediate charge loss by facilitating intersystem crossing between the singlet and triplet of CT_1, trapping and bimolecular recombination of separated charges via CT_1, and electron back transfer from CT_1 to the polymer triplet. Interestingly, we also observe at the same time efficient charge generation via the CT_1 state. As such, we purpose a dual role of CT_1 in both charge loss and charge generation. We furthermore suggest the physical principle and possible pathways to turn CT_1 from a loss channel into a charge generation channel.

+ Author for correspondence: wmc@ifm.liu.se

9:15am **PCSI-ThM-10 2D Materials: Surfaces, Interfaces, and Defects**, ***Robert Wallace,*** University of Texas at Dallas **INVITED**

The size reduction and economics of integrated circuits, captured since the 1960's in the form of Moore's Law, is under serious challenge. Current industry roadmaps reveal that physical limitations include reaching aspects associated with truly atomic dimensions, and the cost of manufacturing is increasing such that only 2 or 3 companies can afford leading edge capabilities. To address some of the materials physical limitations, "2D materials" such as graphene, phosphorene, h-BN, and transition metal dichalcogenides have captured the imagination of the electronics research community for advanced applications in nanoelectronics and optoelectronics. Among 2D materials "beyond graphene," some exhibit semiconducting behavior, such as transition-metal dichalcogenides (TMDs), and present useful bandgap properties for applications even at the single atomic layer level. Examples include "MX_2", where M = Mo, W, Sn, Hf, Zr and X = S, Se and Te

In addition to the potentially useful bandgaps at the monolayer thickness scale, the atomically thin layers should enable thorough electric field penetration through the channel, thus enabling superior electrostatic control. Further, with such thin layers, the integration with suitable gate dielectrics can result in a mobility enhancement. From an interface perspective, the ideal TMD channel material should have a dearth of dangling bonds on the surface/interface, resulting in low interface state densities which are essential for efficient carrier transport. The ideal TMD materials have much appeal, but the reality of significant densities of defects and impurities will surely compromise the intrinsic performance of such device technologies. This presentation will examine the state-of-the-art of these materials in view of our research on semiconductor device applications, and the challenges and opportunities they present for electronic and optoelectronic applications.[1]

This work is supported in part by the SWAN Center, a SRC center sponsored by the Nanoelectronics Research Initiative and NIST. It is also supported in part by Center for Low Energy Systems Technology (LEAST), one of six centers supported by the STARnet phase of the Focus Center Research Program (FCRP), a Semiconductor Research Corporation program sponsored by MARCO and DARPA, the US/Ireland R&D Partnership (UNITE) under the NSF award ECCS-1407765, and the Erik Jonsson Distinguished Chair.

[1] S. J. McDonnell and R.M.Wallace, *Thin Solid Films*, **616**, 482-501 (2016).

9:45am **PCSI-ThM-16 Synthesis, Properties and Tunability of Lateral 2D Heterostructures**, ***Shruti Subramanian,*** *D Deng,* The Pennsylvania State University*; K Xu,* University of Pittsburgh*; N Simonson, K Wang,* The Pennsylvania State University*; J Li, R Feenstra,* Carnegie Mellon University*; S Fullerton-Shirey,* University of Pittsburgh*; J Robinson,* The Pennsylvania State University

Heterogenous combinations of two-dimensional (2D) layered materials provides us with an ability to tune properties tailored for specific applications. Transition metal dichalcogenides (TMDs) are attractive 2D materials in the "beyond graphene" realm of materials. Low resistance contacts are instrumental to utilize their unique electronic properties. Graphene is a promising candidate and has been shown to produce low-resistance contacts to a few TMDs[1] via manual stacking. We have developed a reproducible method to grow lateral heterostructures of graphene and TMDs like MoS_2, thus allowing for the graphene to be used like an "as-grown" near-Ohmic contact[2]. Here, we discuss electronic properties resulting from the interface of these as-grown lateral hetero-structures.

Cross sectional high-resolution transmission electron microscopy is able to demonstrate that the actual interface is a vertical overlap (a few hundred nms) of the MoS_2 onto the edge of the graphene pattern. The van der Waals stacking is maintained at the interface, leading to a pristine and unique combination, which allows for the reduced contact resistance to MoS_2 using graphene as the contacting material instead of conventional metals like Ti/Au. The flexibility of being able to tune the doping of the epitaxial graphene allows us to explore the option of type-matching the graphene contact to the TMD, thus reducing the barrier for electrons and making contacts much superior to conventional metals. This study also explores the impact of this interface in electronic band alignments via low energy electron reflectivity and temperature dependent current measurements.

[1] Das, S. *et al.Nano Lett.***14,** 2861–2866 (2014). [2] Subramanian, S. *et al.* Carbon (Accepted, 2017)

9:50am **PCSI-ThM-17 Surface Potential and Photoresponsive Behavior at Graphene-Metal Interfaces**, ***Matthew DeJarld,*** *P Campbell, A Friedman, M Currie, R Myers-Ward, A Boyd, S Rosenberg, S Pavunny,* U.S. Naval Research Laboratory*; K Daniels,* University of Maryland*; K Gaskill,* U.S. Naval Research Laboratory

Graphene has remarkable photonic properties and, combined with its exceptional electronic transport properties, has led to a number of unique photonic devices.[1-3] Among these are photodetectors utilizing the photo thermoelectric effect, where devices are fabricated having metal contacts with differing work functions.[2,3] Yet, since metals contact-dope graphene, the (unintentional) formation of junctions at the edge of each contact may increase contact resistance as well as generate a photoresponse when illuminated. Despite the ubiquitous presence of metal junctions in all device types, little work exists that describes the behavior of non-noble metals on graphene. Hence, we present a preliminary study of the interactions between graphene and wide range of metals.

Here, we measure the work function, of a wide variety of metals deposited on monolayer epitaxial graphene synthesized on SiC. We find a discrepancy between the measured and reported work functions of metals traditionally considered to have low values, with the work function measured on graphene being consistently higher. We also characterize the films with photovoltage and Raman spectroscopy. For example, Yb films exhibit the strongest photovoltage response despite having a modest work function, and we identify several metals having significant adhesion issues to graphene. In addition, Eu films on graphene have unique phonon signatures with strong Raman peaks at high energies (>1900cm^{-1}) in the spectrum. These peaks may be due to Eu-adsorption within the graphene lattice.[4] A closer look at the graphene-metal interface of Er films via Raman Spectroscopy (Fig. 1) shows evidence of disorder in the graphene lattice at the metal-graphene-air contact point, suggesting bonding with the graphene lattice may occur during oxidation. Such interactions are candidates to influence electronic transport across graphene-metal contacts.

References

[1] K. F. Mak, et al. *Physical Review Lettersm* **101**, 196406 (2008).

[2] T. Mueller, F. Xia, and P. Avouris. *Nature Photonics* **4**, 297 (2010).

[3] C. Xinghan, et al. *Nature Nanotechnology* **9**, 814 (2014).

[4] D. Förster, et al. *New Journal of Physics* **14**, 023022 (2012).

10:30am **PCSI-ThM-25 Force Measurement by Atomic Force Microscopy with a Molecular Tip at Low Temperature**, ***Shigeki Kawai,*** National Institute for Materials Science, Japan **INVITED**

Recent progress in atomic force microscopy allows us to see inner structures of molecules adsorbed on surfaces [1]. In such measurements, a reactive metal tip is usually terminated by a small molecule or an inert rare gas atom. Such high-resolution imaging is beneficial to study single and self-assembled molecules as well as chemical reactions. Besides high-resolution imaging, force measurements became more reliable and even quantitative since the structure of the tip apex, at least the front-most-atom, can be controlled in experiment.

In this presentation, force spectroscopic measurements with different molecular tips (i.e. Xe-tip for van der Waals force detection [2] and CO-tip for the intermolecular bond detection [3]) will be discussed (Fig. 1). Besides the small atom and molecule, the tip can be also terminated with a large molecule or a polymer. By moving the tip vertically, we measured desorption phenomena of repeat polyfluorene units [4]. We found that the incommensurability between the unit length and the lattice distance plays a role in the friction. Since the fluorene units are connected to each other by a single bond, the incommensurability is not high. Using a stiffer material in-plane, a lower friction can be expected. In fact, the super lubricity was detected when graphene nanoribbon was slid on Au(111) [5].

[1] L. Gross, F. Mohn, N. Moll, P. Liljeroth, and G. Meyer, *Science*, **325**, 1110 (2008).

[2] S. Kawai, A. S. Foster, T. Björkman, S. Nowakowsaka, J. Björk, F. Federici Canova, L. H. Gade, T. A. Jung, and E. Meyer, *Nature Communications*, **7**, 11559 (2016).

[3] S. Kawai, T. Nishiuchi, T. Kodama, P. Spijker, R. Pawlak, T. Meier, J. Tracey, T. Kubo, E. Meyer and A. S. Foster, *Science Advances***3**, e1603258 (2017).

[4] S. Kawai, M. Koch, E. Gnecco, A. Sadeghi, R. Pawlak, Th. Glatzel, J. Schwarz, S. Goedecker, S. Hecht, A. Baratoff, L. Grill, and E. Meyer, *Proc. Natl. Acad. Sci. USA* 111, 3968 (2014).

[5] S. Kawai, A. Benassi, E. Gnecco, H. Söde, R. Pawlak, K. Mullen, D. Passerone, C. Pignedoli, P. Ruffieux, R. Fasel, and E. Meyer, *Science*, **351**, 957 (2016).

11:00am **PCSI-ThM-31 Local Deep Level Transient Spectroscopy Imaging for MOS Interface Trap Distribution***, N Chinone,* ***Yasuo Cho****,* Tohoku University, Japan

Physical properties of metal-oxide-semiconductor (MOS) interface are critical for semiconductor devices. There are several techniques for characterizing MOS interface properties. Deep level transient spectroscopy (DLTS) [1] is one of powerful techniques capable of macroscopic quantitative evaluation of trap density at/near MOS interface. But it is easily imagined that actual trap is not homogeneously distributed but has two dimensional distributions in atomic scale and even in mesoscopic scale. Therefore, it is very important to characterize MOS interface microscopically. Unfortunately, it is impossible to observe such inhomogeneity by using conventional macroscopic DLTS method.

In this paper, a new technique for local DLTS imaging using scanning nonlinear dielectric microscopy (SNDM) [2] is proposed. This method enables us to observe two dimensional distribution of trap density at/near MOS interface and is demonstrated with oxidized SiC wafer.

We measured three n-type silicon face (4°-off) 4H-SiC wafer samples on which 45-nm-thick thermal silicon dioxide film was formed. Two of them were followed by post oxidation annealing (POA) in nitric oxide ambient with different annealing conditions: (a) 10 min in 1250°C and (b) 60 min in 1150°C. We labeled the samples without POA, with POA in condition (a) and with POA in condition (b) as #S-45-1, #S-45-2 and #S-45-3, respectively. These three samples were scanned on $1.5\times1.5mm^2$ square area with a resolution of 30×30 pixels and analyzed using the proposed local DLTS method. By analyzing the acquired images, time-constant and magnitude of transient capacitance response were obtained at each pixel. As shown in Figure 1, highest brightness was obtained from #1 and lowest one was obtained from #3, which is consistent with macroscopically obtained result (#1 sample has highest trap density and #3 sample has lowest one.). Furthermore, in the local DLTS images, we detected dark and bright areas, which can be translated as two dimensional trap distribution. This means that this is the first demonstrations of two dimensional imaging of trap distributions in MOS interfaces.

+ Author for correspondence: yasuocho@riec.tohoku.ac.jp

[1] D. V. Lang: J. Appl. Phys. **45**,3023 (1974).

[2] Y. Cho et al.: Rev. Sci. Instrum. **67**, 2297(1996).

11:15am **PCSI-ThM-34 Interaction and Topological Effects in Two-dimensional Materials***, Steven G. Louie,* UC Berkeley **INVITED**

Symmetry, interaction and topological effects, as well as environmental screening, dominate many of the quantum properties of reduced-dimensional systems and nanostructures. These effects often lead to manifestation of counter-intuitive concepts and phenomena that may not be so prominent or have not been seen in bulk materials. In this talk, I present some fascinating physical phenomena discovered in recent studies of atomically thin two-dimensional (2D) materials. A number of highly interesting and unexpected behaviors have been found – e.g., strongly bound excitons (electron-hole pairs) with unusual energy level structures and novel optical selection rules; massless excitons; tunable magnetism and plasmonic properties; electron supercollimation by disorders; and novel topological phases – adding to the promise of these 2D materials for valuable applications.

Author Index

Bold page numbers indicate presenter